2,6-Pyridinedicarboxylic acid, dodecyl phenethyl ester

Inchi: InChI=1S/C27H37NO4/c1-2-3-4-5-6-7-8-9-10-14-21-31-26(29)24-18-15-19-25(28-24)27(

InchiKey: PZOXBIJASZIILU-UHFFFAOYSA-N

Formula: C27H37NO4

SMILES: CCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCCc2ccccc2)n1

Mol. weight [g/mol]: 439.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.36		Crippen Method
logp	6.559		Crippen Method
mcvol	368.630	ml/mol	McGowan Method
rinpol	3244.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U369230&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices